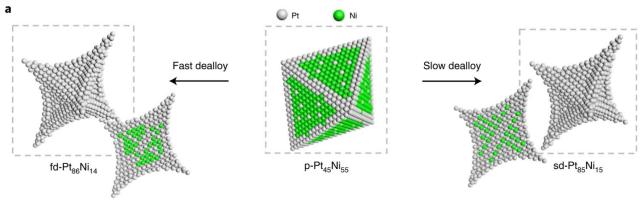
Predicting the Durability and **Activity for Pt Catalysts**









Scientific Achievement

Scientists have shown that essential x-ray absorption spectral features correlate with the fine structure of Pt alloys and can be used as a descriptor to predict both the activity and stability of the catalysts.

Significance and Impact

The adoption of proton-exchange fuel cells is hindered by the lack of predictability of highly active and durable platinum-based catalysts for accelerating the sluggish oxygen reduction reaction. This work opens a way to uncover the missing information.

A dealloying process is used to form Pt-alloy catalysts with similar morphologies and compositions. The descriptor proposed in this work can predict their different activities and stabilities.

J. Huang, L. Sementa, Z. Liu, G. Barcaro, M. Feng, E. Liu, L. Jiao, M. Xu, D. Leshchev, S.–J. Lee, M. Li, C. Wan, E. Zhu, Y. Liu, B. Peng, X. Duan, W. A. Goddard III, A. Fortunelli, Q. Jia, Y. Huang. *Nature Catalysis* **5**, 513–523 (2022).

This work was performed at the National Synchrotron Light Source II.

Research Details

- Developed a binary experimental descriptor that captures strain and Pt transition metal coupling contributions through x-ray absorption spectroscopy at the BMM, ISS, and QAS beamlines at NSLS-II.
- Correlated theoretical modelling and experimental observations for predicting the catalytic activity and stability.
- This method can be transferred to a wide range of Pt-alloy oxygen reduction reaction catalysts.











